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ABSTRACT

It has been recently reported that the electrical charge in a semiconductive carbon nanotube is not evenly distributed, but is divided into charge "islands [1,2]." A clear understanding of tunneling phenomena can be useful to elucidate the mechanism for electrical conduction in nanotubes. This paper represents the first attempt to shed light on the aforementioned phenomenon through viewing tunneling as a natural consequence of "discrete trajectories." The relevance of this analysis is that it may provide further insight into the higher rate of tunneling processes, which makes tunneling devices attractive [3]. In a situation involving particles impinging on a classically impenetrable barrier, the result of quantum mechanics that the probability of detecting transmitted particles falls off exponentially is derived without wave theory. This paper should provide a basis for calculating the charge profile over the length of the tube so that nanoscale devices' conductive properties may be fully exploited.

1 INTRODUCTION

This introduction serves as an outline for the paper. The idea of the "warp tunnel" is essential for subsequent calculations in this paper. Though it sounds futuristic, the idea is straightforward and sound. The warp tunnel is introduced in Figure 1. Its quantitative properties are explored in Figure 2, which attempts to provide insight into the higher rate of tunneling processes. Figure 3 hints at the explanation of the charge island phenomenon, and also provides a basis for understanding subsequent calculations. To show the potency of this analytical model, we calculate the transmission probability of a beam of electrons impinging on a classically impenetrable barrier, the scenario shown in Figure 4. Having successfully obtained the result, we look within the analysis to obtain the explanation for charge islands.

2 BACKGROUND AND MOTIVATION

We begin with consideration of Figure 4. Electrons emitted from a source S impinge on a potential barrier. To penetrate the barrier, they must tunnel a distance a while bridging the distance r. We wish to find p(L), or the probability of bridging the distance r while traveling only L = r − a. In Figure 5, we visualize distance r as consisting of warp tunnels of differing constituents. Uncharged particles are shown as white while electrons are black.

Although the number of electrons in each warp tunnel increases from top to bottom in this figure, such an arrangement is solely for conceptual simplicity. The number of electrons pictured in each warp tunnel symbolizes the number of electrons involved in the momentum transfer to the outgoing electron in each warp tunnel. It is assumed that the greater the involvement of uncharged particles in the momentum transfer, the faster the transfer will occur, owing to the greater size of the uncharged particles.

Figure 6 shows that the uncharged particles move but little in a chain reaction or momentum transfer, but the electrons, being smaller, must move more to propagate the chain reaction. When particle A, in Figure 6, is inserted into the warp tunnel in (I), its representative exits almost immediately. The effective distance traveled by A is on the order of its diameter. However, when A is inserted into warp tunnel (II), its effective distance traveled is greater.

2.1 Model Verification Calculation

To formalize the calculation, it is assumed that the mean free path of an electron is d, while that of an uncharged particle is 0. In warp tunnel (a) of Figure 5, it is presumed that an incoming electron will travel d once it enters the tunnel, collide with an uncharged particle, which will then transfer that momentum via other uncharged particles to an outgoing electron, which will exit the warp tunnel almost immediately after the first electron entered it. As depicted in Figure 3, such a scenario becomes increasingly improbable as the length of the warp tunnel increases. In warp tunnel (b) of Figure 5, since the mean free path of uncharged particles is 0 and the current flows to the left, we may assume that the electron inside the tunnel is flushed to the right of its adjacent uncharged particle on its left. That electron then having a mean free path of d has to its immediate right a distance d of intervening space separating it from the next uncharged particle in the tunnel. So the incoming electron travels a distance d once it enters the tube, transfers its momentum to the uncharged particles, which cause the middle electron to travel through a distance d, which was to its right. It collides with uncharged particles, which cause an electron to be ejected from the warp tunnel. The amount of time it takes to eject an electron after one has entered in warp tunnel (b) is about twice that in warp tunnel (a). A convenient abstraction is to regard an electron entering a tunnel as appearing for a few instants, disappearing, and reappearing at a point further downstream the tunnel. The more "appearances" an electron makes in a tunnel, the longer its trip through the tunnel. Here enters the

notion of a "discrete trajectory." The electron does not travel continuously through the tube, but successively appears at subsequent points in the tube and disappears between those points.

In Figure 5, i - 1 electron mean free path domains are evenly distributed throughout the warp tunnel. This assumption is true on average. For a warp tunnel with L = i d, we calculate p(L) as follows. To choose i - 1 domains out of the interval [-r,0] as free path positions for the i - 1 electrons, we recognize that the number of points from which to choose is n = r/d. The number of ways of obtaining a warp tunnel with L = i d, is n (n - 1) (n - 2) ...(n - (i - 2)) = n!/(n - (i - 1))! We use Stirling's Formula to simplify.

$$p(L) \propto 1/(n - (i - 1))!$$

$$p(L) \propto e^{-[(n - i + 2) + (n - i + \frac{1}{2}) Ln(n - i + 2)]}.$$

$$L = i\, d \Rightarrow i = L/d,\ n - i = (r - L)/d.$$

$$p(L) \propto G \cdot e^{k L}.$$

The probability of detecting electrons on the other side of the barrier requires L = r - a, and is given by:

$$p(L) \propto e^{-[a/d + (a/d + \frac{1}{2}) Ln(a/d + 2)]}.$$

If a/d >> 1, p(L) → 0 very quickly, but if a/d ≈ 1,

$$p(L) = G\, e^{-k' a},$$

which falls off exponentially with increasing barrier width a. G and the k are independent of r.

3 MODEL EXPLOITATION

The calculation of the charge separation is lengthy and involved. Consequently, only general remarks, an outline of the calculation and reporting of those results appear here. The idea behind charge islands is closely associated with that of mean free path. A free-floating electron travels by a certain average amount before it collides with another particle, possibly dislodging an electron and imparting it with its motion. The electron need not directly bump into another electron though. It may transfer its motion by bumping into several intervening neutral particles. Tunneling viewed in this light is to induce the motion of a distinct, yet otherwise indistinguishable, particle indirectly via intervening, and possibly different, particles—much in the same way as making a combination shot in pool. Charge islands are formed at regular intervals due to the chain-reaction creation of charged particles a certain mean distance from an immediately upstream impulse due to the indirect motion of charged particles there. We may think of a length L nanotube as a warp tunnel containing i electron islands. These islands will be evenly spaced on average. In a nanoscale metallic conductor, the spacing of the charge islands is so close that the charge appears to be uniformly distributed. However, in a nanoscale semiconductor, the spacing of charge islands increases, revealing charge granularity.

3.1 Spacing Calculation Outline

Since charge is segregated into islands, to model this circuit, an appropriate technique seems to be that of the series RC circuit. A capacitor plate represents a charge island; the spacing between the plates of the capacitor represents the neutral gaps between adjacent charge islands. The capacitors are modeled as having equal capacitance while R represents the internal resistance of the circuit. Ordinarily, we would not expect a capacitor to conduct a DC current, but if the plate spacing is sufficiently close a tunneling current will flow in the same way that electrons will pass through the barrier shown in Figure 4 if a is small enough. When tunneling is viewed in this new light, a tunneling current can readily transmit through 40 nm barriers.

Consider the warp tunnel in the top of Figure 1. Ignoring its coloring, let the particle entering the tunnel be a photon emitted by an electron, not displayed, to its left. Assume that the warp tunnel spans a barrier of width a. The particle emerging from the right side of the warp tunnel may be a photon that will be absorbed by an electron, not displayed, on the right side of the barrier. The outgoing photon thereby imparts that electron with the motion originally possessed by the other electron on the left side of the barrier. In these calculations, it is assumed that the photon has a width, denoted lt, directly proportional to its energy or frequency. The proportionality constant is derived from physical constants.

Assuming the warp tunnel in Figure 1 is full, the entering photon need only move into the tunnel an amount lt when a representative photon will move out of the tunnel. The electron, which originally emitted the photon, has effectively bridged the distance across the barrier by "traveling" only a distance lt << a. The effective length of the barrier is only lt(f), or the width of the photon of frequency f perpetuating the motion. This analysis explains both the optical and quantum mechanical barrier penetration phenomena shown in Figure 7. In general, it is not the selfsame electron that impinges on the barrier in Figure 7.a that emerges on the other side. Likewise, it is not the selfsame photon that enters the prism on the left that is detected beyond the prism on the right.

This model allows one to conclude that the effective length of the barrier may be given by the width, lt(f), of a photon within the barrier. To find the probability distribution function, f(L), of the length of the barrier, we use the Planck distribution function, which gives the thermal average number of photons in a single mode of frequency. For the temperature variable, we use room temperature. The majority of the frequencies are smaller

than that of visible light; hence, f(L) ∝ 1/L, where L is a function of frequency.

We return now to our classical RC circuit model. When the power is turned on in a classical DC RC circuit, we obtain a transient solution: a current that exponentially decays in time. However, if the capacitor plate spacing is not fixed, but is exponentially decreasing with increasing time, we find that the current through the capacitor is essentially constant and inversely exponentially depends on the original plate spacing. The probability distribution function, g(L), of the length L between the capacitor plates, or the plate spacing, must give g(L) ∝ 1/L to explain a plate spacing that exponentially decays with time. This remarkable and highly convincing result shows that harmony may be obtained between standard tunneling current formulae and that predicted by DC RC circuit analysis by assuming that the tunneled current follows a discrete trajectory across the barrier.

Detailed calculations were performed to obtain the coefficient of time in the decreasing exponential factor involved in the plate spacing of the capacitor. This value, along with the internal resistance of the circuit, is needed to resolve the formula for the tunneling current through the nanotube circuit or the tunneling resistance of the nanotube.

This model reasonably predicts the charge separation contingent on one measurement, which was not reported in the literature discussing this phenomenon: the internal resistance of the circuit when the semiconducting nanotube is short-circuited by a metallic nanotube or another extremely low resistance shunt. So, if the power supply were shut off, and the two nanotube terminals, gold in one test and platinum in another, were short-circuited by an extremely low resistance shunt and a highly sensitive ohmmeter were placed in series, one lead at the positive terminal of the power supply and one at the negative terminal of the power supply, the resistance, R, that the ohmmeter would read for the two scenarios reported in [2]—keeping all things constant such as temperature, the length of the tubes, the length and composition of the leads to the tubes, and identical final charge spacing—is needed.

An equivalence is established which allows calculation of the charge separation based on traditional circuit parameters yielded readily from macroscopic measurements and the literature. We equate the tunneling resistance of the entire nanotube with no islands at t = 0 when the power supply is switched on to that which would result from an arbitrary number n of charge islands which are manifested at t > 0. Solving for n yields the number of charge islands, which the model says should be evenly spaced. Knowledge of the length of the nanotube gives the separation of the charge islands. The charge separation for various R has been calculated and is presented below:

4 RESULTS

Results are given in the form: (R in Ohms, charge island spacing in nm). For the 650 nm tube, (0.0001270, 37.7), (0.0001316, 42.6), and (0.0001292, 40). For the 750 nm tube, (0.0001370, 34.4), (0.0001408, 37.82), and (0.0001389, 36). These resistances seem in range. They are just what one would expect of the resistances of the leads in these experiments.

5 REMARKS

A general observation about tunneling is that as the mass or equivalent energy of a tunneled particle decreases, the greater its transmission probability. When we apply this analysis to the optical experiment in Figure 7, we see that d is on the order of the wavelength of the incident light. Observe that lower frequency electromagnetic radiation has greater penetrating ability, which also may be related to the size of its photons. As a final comment, a standing wave may be thought of as existing inside the potential barrier in Figure 4. Analogously, this "island," phenomenon may also exist on a macroscopic scale and may be manifested with light in microwave ovens, which often do not heat food uniformly, but leave hot and cold spots in food.

6 CONCLUSIONS

A theoretical framework was introduced to better understand tunneling. It was successfully applied to determine the transmission probability of a stream of electrons incident on a potential barrier. An appeal was made to the established model to help explain the reported phenomenon of charge separation in carbon nanotubes.

Calculations have been performed which show that while to calculate the capacitance above the nanoscale, the plate spacing d(t) of a capacitor should be a fixed constant, independent of time, at the nanoscale, d(t) rapidly decreases as a function of time in accordance with the probability distribution function—predicted by this theory—of the lengths of the discrete trajectories of electrons bridging the gap of the capacitor. When this calculation is performed, an equation—identical in form to that of Giaever—yielding the current through the circuit as an inverse exponential function of the original plate spacing of the capacitor is obtained. This equation is then used to obtain the spacing of the charge islands. The fact that the classical equations for a series RC circuit can still be utilized on the nanoscale by assuming the plate spacing of the capacitor is shrinking by a function of time which is predicted by this theory is strong proof alone that this theory is sound.

General remarks about tunneling with light and electrons were made with the implication that the phenomenon of tunneling is more ubiquitous than perhaps generally thought. The theoretical model seems accurate and was inspired by a more general computer program written by the author.
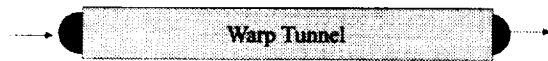
Warp Tunnel

The elapsed time to push a particle into the warp tunnel is the amount of time it takes for "it" to completely emerge at the other end, independent of the length of the tunnel.

Cutaway View of Warp Tunnel

The particle emerging as a consequence of tunnel overflow is not the selfsame particle inserted, but to the extent that subatomic particles are indistinguishable, it represents the particle inserted.

Figure 1: The warp tunnel.
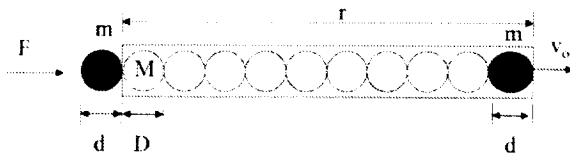
$F = M (r/D) g'$, where g' is the acceleration due to F.
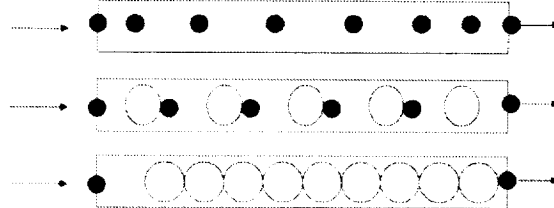$d = g' t^2/2$, $t = (2 d/g')^{0.5}$
$v_1 = (r + d)/t = (r + d) (F/(2 d M (r/D)))^{0.5}$
Instead of F acting on a particle, assume it has a corresponding initial input v_i, then "it" will effectively traverse tunnel with v_1.
$m v_i^2/2 = F d$, $v_i = (2 F d/m)^{0.5}$
$v_1/v_i = (r + d)/(2 d M (r/D))^{0.5} (m/(2 d))^{0.5}$
$= (r + d) (m D)^{0.5}/(2 d)/(M r)^{0.5}$
$\approx 0.5 (r/d) (m/M)^{0.5} (D/r)^{0.5}$, if $r >> d$. $v_o \leq v_1$.

Figure 2: Higher rate of tunneling processes.

White particles are uncharged while black ones are charged.
Separations near charged particles are of a distance quantum, which may exceed the particle diameter.
For warp tunnels of a certain equal length, the probability of each of the three pictured scenarios decreases from top to bottom.

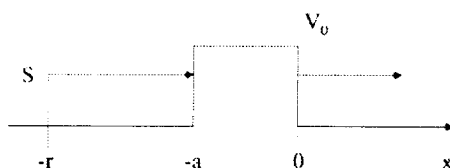Figure 3: Warp scenarios.

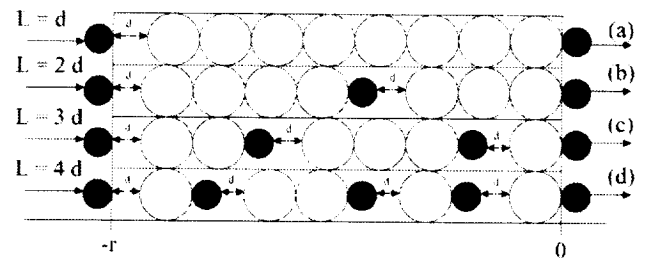Figure 4: Stream on potential barrier.
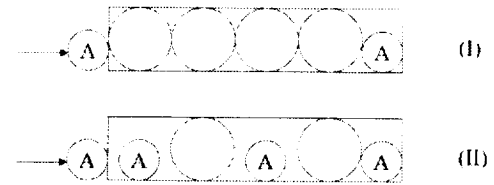

Figure 5: Warp tunnel constituents.

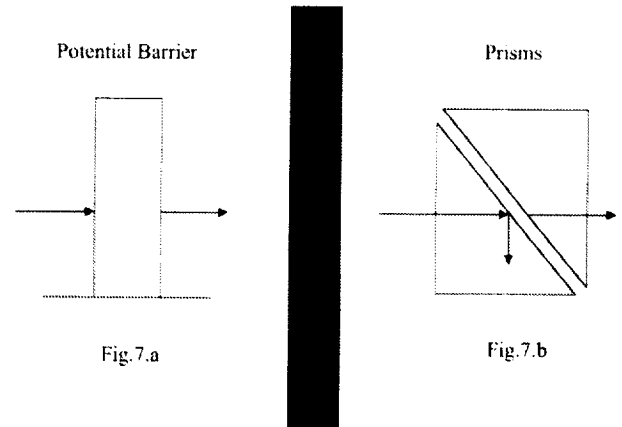Figure 6: Size influences warp effect.

Figure 7: Optical and quantum mechanical tunneling.

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[1] G. Khitrov, "Carbon nanotubes electric charge divides into charge 'islands,'" MRS BULLETIN, pp. 4-5, July, 2000.
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[3] Linda Geppert, "Quantum transistors: toward nanoelectronics," IEEE Spectrum, pp. 46-51, September, 2000.

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